

# Momentum Dependent Local-Ansatz Wavefunction from Weak to Strong Electron Correlations

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Momentum dependent local-ansatz (MLA) wavefunction describes accurately electron correlations from the weak to intermediate Coulomb interaction regimes. We point out that the MLA can describe the correlations from the weak to strong Coulomb interaction regimes by modifying the starting wavefunction from the Hartree-Fock (HF) type to an alloy-analogy (AA) type wavefunction. Numerical results based on the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions show up that the new wavefunction yields the ground-state energy lower than the Gutzwiller wavefunction (GW) in the whole Coulomb interaction regime. Calculated double occupation number is smaller than the result of the GW in the metallic regime, and is finite in the insulator regime. Furthermore, the momentum distribution shows a distinct momentum-dependence in both the metallic and insulator regions, which are qualitatively different from those of the GW.

**KEYWORDS:** variational method, electron correlations, Gutzwiller wavefunction, local ansatz, Hubbard model, metal-insulator transition, critical Coulomb interaction, infinite dimensions

The variational theory is a useful tool for studying the ground-state properties of correlated electron system such as the magnetism, the heavy-electron behavior, the metal-insulator transition, and the high-temperature superconductivity.<sup>1–16)</sup> There the form of the wavefunction is crucial to describe electron correlations. The Gutzwiller wavefunction (GW) is one of the popular wavefunctions, because of its simplicity and applicability to realistic systems.<sup>1–3)</sup> It describes electron correlations by making use of a projection operator  $\Pi_i(1 - g\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$  onto the Hartree-Fock (HF) wavefunction  $|\phi_0\rangle$ ;

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$|\Psi_{\text{GW}}\rangle = [\prod_i (1 - g \hat{n}_{i\uparrow} \hat{n}_{i\downarrow})] |\phi_0\rangle$ . Here  $\hat{n}_{i\sigma}$  is the number operator for an electron on site  $i$  with spin  $\sigma$ , variational parameter  $g$  reduces the amplitudes of doubly occupied states on local orbitals. The local-ansatz approach (LA) proposed by Stollhoff and Fulde is an alternative method which is simpler than the GW.<sup>4–7)</sup> The LA wavefunction takes into account the states expanded by the residual Coulomb interactions  $\{O_i\} = \{\delta \hat{n}_{i\uparrow} \delta \hat{n}_{i\downarrow}\}$ ;  $|\Psi_{\text{LA}}\rangle = [\prod_i (1 - \eta_{\text{LA}} O_i)] |\phi_0\rangle$ . Here  $\delta \hat{n}_{i\sigma} = \hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle_0$ ,  $\langle \hat{n}_{i\sigma} \rangle_0$  being the HF average of electron number on site  $i$  with spin  $\sigma$ . The amplitude  $\eta_{\text{LA}}$  is determined variationally.

Although the GW and the LA have been applied to a number of correlated electron systems, they are not sufficient for the description of correlations from the weak to strong interaction regimes. In fact, both the GW and the LA do not describe exactly the weakly correlated regime due to the use of limited Hilbert-space. Furthermore in the strong Coulomb interaction regime, the GW yields the Brinkman-Rice atom (*i.e.*, no charge fluctuation on an atom) instead of the insulator solid in infinite dimensions ( $d = \infty$ ).<sup>17)</sup> In order to overcome the difficulty in the weak Coulomb interaction regime and to improve the behaviors in the intermediate Coulomb interaction regime, we have recently proposed the momentum-dependent local ansatz wavefunction (MLA).<sup>18,19)</sup> The MLA wavefunction controls the amplitudes of momentum-dependent two particle states to be best, and much improves the Fermi liquid properties of the GW and the LA in those regimes.

The wavefunction which accurately describes the strong Coulomb interaction regime has been proposed by Baeriswyl.<sup>9–12)</sup> The Baeriswyl wavefunction (BW) is constructed by applying a hopping operator  $\hat{T}$  onto the atomic wavefunction  $|\Psi_\infty\rangle$ ;  $|\Psi_{\text{BW}}\rangle = e^{-\eta \hat{T}} |\Psi_\infty\rangle$ . Here  $\hat{T} = - \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma}$  is the kinetic energy operator.  $t_{ij}$  denotes the transfer integral between sites  $i$  and  $j$ ,  $a_{i\sigma}^\dagger$  ( $a_{i\sigma}$ ) being the creation (annihilation) operator for an electron on site  $i$  with spin  $\sigma$ . The operator  $e^{-\eta \hat{T}}$  with a variational parameter  $\eta$  describes electron hopping from the atomic state and suppresses the configurations with high kinetic energy. Although the BW describes well the insulator state in the strong correlation regime, it is not easy to describe the metallic state from this viewpoint. There is no other variational wavefunction which is suitable for both the weak and strong Coulomb interaction regimes and can be analytically treated, as far as we know.

In this letter, we point out that a modified MLA wavefunction which starts from the alloy-analogy (AA) wavefunction instead of the HF one describes the strongly correlated regime reasonably so that one can go beyond the GW in both the weak and strong

Coulomb interaction regimes. The wavefunction provides us with a new tool to describe various systems with intermediate Coulomb interaction strength such as the cuprates and the iron pnictides superconductors.

We adopt in this letter the single-band Hubbard model as follows:<sup>1, 20, 21)</sup>

$$H = \sum_{i\sigma} (\epsilon_0 - \mu) \hat{n}_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \quad (1)$$

Here  $\epsilon_0$  ( $\mu$ ) is the atomic level (chemical potential),  $t_{ij}$  is the transfer integral between sites  $i$  and  $j$ .  $U$  is the intra-atomic Coulomb energy parameter.

The construction of the MLA wavefunction is rather simple. We expand first the LA wavefunction up to the first order with respect to the Coulomb interaction strength  $U$  and observe that each coefficient of the two-particle excited states in the first-order wavefunction is momentum independent in contradiction to the exact result. Therefore, we introduce a new set of local operators  $\{\tilde{O}_i\}$  with the momentum-dependent variational parameters  $\eta_{k'_2 k_2 k'_1 k_1}$  which yields the correct weak Coulomb interaction limit:

$$\tilde{O}_i = \sum_{k_1 k'_1 k_2 k'_2} \langle k'_1 | i \rangle \langle i | k_1 \rangle \langle k'_2 | i \rangle \langle i | k_2 \rangle \eta_{k'_2 k_2 k'_1 k_1} \delta(a_{k'_2 \downarrow}^\dagger a_{k_2 \downarrow}) \delta(a_{k'_1 \uparrow}^\dagger a_{k_1 \uparrow}). \quad (2)$$

Here  $\langle i | k \rangle = \exp(-i\mathbf{k} \cdot \mathbf{R}_i)/\sqrt{N}$  is an overlap integral between the localized orbital and the Bloch state with momentum  $\mathbf{k}$ ,  $\mathbf{R}_i$  denotes atomic position, and  $N$  is the number of sites.  $a_{k\sigma}^\dagger$  ( $a_{k\sigma}$ ) denotes a creation (annihilation) operator for an electron with momentum  $\mathbf{k}$  and spin  $\sigma$ , and  $\delta(a_{k'\sigma}^\dagger a_{k\sigma}) = a_{k'\sigma}^\dagger a_{k\sigma} - \langle a_{k'\sigma}^\dagger a_{k\sigma} \rangle_0$ . We then construct the MLA wavefunction as follows.<sup>18, 19)</sup>

$$|\Psi_{\text{MLA}}\rangle = \prod_i (1 - \tilde{O}_i) |\phi_0\rangle. \quad (3)$$

The best wavefunction is chosen by controlling the variational parameters in the momentum space. Hereafter we refer the wavefunction (3) to the MLA-HF wavefunction.

The MLA-HF wavefunction does suitably describe the electron correlations in the weak and intermediate Coulomb interaction, but it cannot suppress loss of Coulomb repulsion in the strong interaction regime. To improve the difficulty we propose here to change the starting wavefunction from the HF wavefunction to the alloy-analogy (AA) wavefunction which is suitable in the strong Coulomb interaction regime.

The concept of the AA can be traced back to Hubbard's original work on electron correlations.<sup>22)</sup> In the strong Coulomb interaction regime, electrons with spin  $\sigma$  move slowly from site to site due to electron correlations, and therefore should feel a potential  $U$  instead of the HF average potential  $U\langle \hat{n}_{i-\sigma} \rangle_0$ , when the opposite spin electron is on

the same site. Hubbard regarded this system as an alloy with different random potentials  $\epsilon_0 + U$  and  $\epsilon_0$ . The AA Hamiltonian is then defined by

$$H_{\text{AA}} = \sum_{i\sigma} (\epsilon_0 - \mu + Un_{i-\sigma}) \hat{n}_{i\sigma} + \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (4)$$

Since the motion of electrons with opposite spin are treated to be static in the AA approximation, related operators  $\{\hat{n}_{i\sigma}\}$  are regarded as a random static  $C$  number  $n_{i\sigma}$  (0 or 1). Each configuration  $\{n_{i\sigma}\}$  is considered as a snapshot in time development.

We adopt the AA ground-state wavefunction  $\phi_{\text{AA}}$  for the Hamiltonian  $H_{\text{AA}}$ , and propose a new ansatz, which we call the MLA-AA wavefunction, as follows.

$$|\Psi_{\text{MLA-AA}}\rangle = \prod_i (1 - \tilde{O}_i) |\phi_{\text{AA}}\rangle. \quad (5)$$

The local operators  $\{\tilde{O}_i\}$  with variational parameters  $\eta_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1}$  have been modified as

$$\tilde{O}_i = \sum_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1} \langle \kappa'_1 | i \rangle \langle i | \kappa_1 \rangle \langle \kappa'_2 | i \rangle \langle i | \kappa_2 \rangle \eta_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1} \delta(a_{\kappa'_2 \downarrow}^\dagger a_{\kappa_2 \downarrow}) \delta(a_{\kappa'_1 \uparrow}^\dagger a_{\kappa_1 \uparrow}). \quad (6)$$

Here  $a_{\kappa\sigma}^\dagger$  and  $a_{\kappa\sigma}$  are the creation and annihilation operators which diagonalize the Hamiltonian  $H_{\text{AA}}$ , and  $\delta(a_{\kappa'\sigma}^\dagger a_{\kappa\sigma}) = a_{\kappa'\sigma}^\dagger a_{\kappa\sigma} - \langle a_{\kappa'\sigma}^\dagger a_{\kappa\sigma} \rangle_0$ . It should be noted that the MLA-AA wavefunction reduces to the MLA-HF by replacing the random potential  $Un_{i-\sigma}$  with the HF one, *i.e.*,  $U\langle\phi_0|\hat{n}_{i-\sigma}|\phi_0\rangle$ , so that  $\Psi_{\text{MLA-AA}}$  and  $\Psi_{\text{MLA-HF}}$  are mutually connected to each other via a suitable parameter which interpolates between the two wavefunctions.

We can obtain the ground-state energy for the MLA-AA wavefunction within the single-site approximation (SSA) taking the same steps as in the MLA-HF.<sup>18,19)</sup> The correlation energy per atom is then given by

$$\epsilon_c = \frac{-\langle \tilde{O}_i^\dagger \tilde{H} \rangle_0 - \langle \tilde{H} \tilde{O}_i \rangle_0 + \langle \tilde{O}_i^\dagger \tilde{H} \tilde{O}_i \rangle_0}{1 + \langle \tilde{O}_i^\dagger \tilde{O}_i \rangle_0}. \quad (7)$$

Here  $\tilde{H} = H - \langle H \rangle_0$ . Note that the average  $\langle \sim \rangle_0$  is now taken with respect to the AA wavefunction. The total energy per atom should be obtained by taking the configurational average;  $\langle H \rangle = \overline{\langle H \rangle_0} + N\overline{\epsilon_c}$ . Here the upper bar denotes the configurational average. Each term in the correlation energy can be calculated by making use of Wick's theorem.

We obtain a self-consistent equation with variational parameters using the minimum energy condition.

$$(\Delta E_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1} - \epsilon_c) \eta_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1}$$

$$\begin{aligned}
& + \frac{U}{N^2} \left[ \sum_{k_3 k_4} f(\tilde{\epsilon}_{\kappa_3 \uparrow}) f(\tilde{\epsilon}_{\kappa_4 \downarrow}) \eta_{\kappa'_2 \kappa_4 \kappa'_1 \kappa_3} - \sum_{\kappa_3 \kappa'_4} f(\tilde{\epsilon}_{\kappa_3 \uparrow}) (1 - f(\tilde{\epsilon}_{\kappa'_4 \downarrow})) \eta_{\kappa'_4 \kappa_2 \kappa'_1 \kappa_3} \right. \\
& \left. - \sum_{\kappa'_3 \kappa_4} (1 - f(\tilde{\epsilon}_{\kappa'_3 \uparrow})) f(\tilde{\epsilon}_{\kappa_4 \downarrow}) \eta_{\kappa'_2 \kappa_4 \kappa'_3 \kappa_1} + \sum_{\kappa'_3 \kappa'_4} (1 - f(\tilde{\epsilon}_{\kappa'_3 \uparrow})) (1 - f(\tilde{\epsilon}_{\kappa'_4 \downarrow})) \eta_{\kappa'_4 \kappa_2 \kappa'_3 \kappa_1} \right] = U . \quad (8)
\end{aligned}$$

Here  $\Delta E_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1}$  is the two-particle excitation energy given by  $\Delta E_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1} = \epsilon_{\kappa'_2 \downarrow} - \epsilon_{\kappa_2 \downarrow} + \epsilon_{\kappa'_1 \uparrow} - \epsilon_{\kappa_1 \uparrow}$ .  $\epsilon_{\kappa \sigma}$  denotes one-electron eigen value energy for  $H_{AA}$ , and  $\tilde{\epsilon}_{\kappa \sigma} = \epsilon_{\kappa \sigma} - \mu$ .  $f(\epsilon)$  is the Fermi distribution function at zero temperature. To solve the equation approximately, we make use of an interpolate solution which is valid in both the weak Coulomb interaction limit and the atomic limit.<sup>18)</sup>

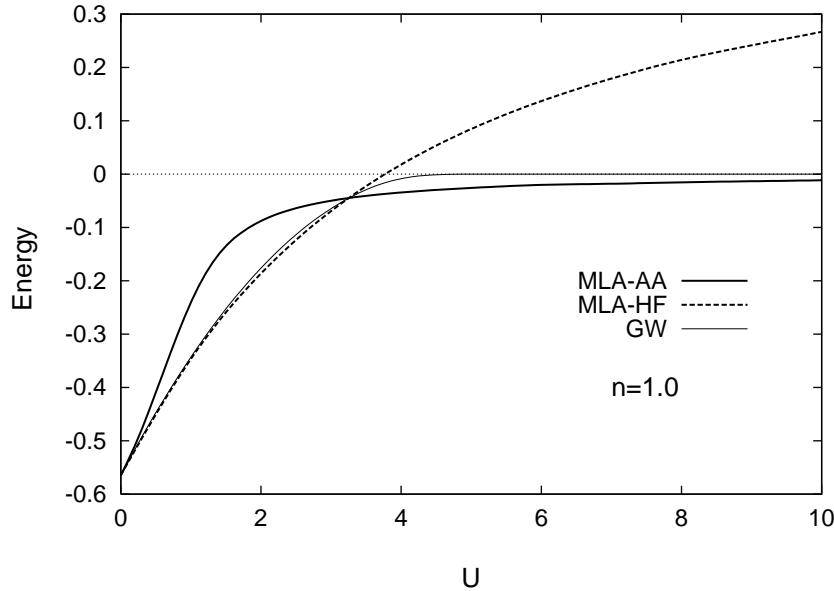
$$\eta_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1}(\tilde{\eta}, \epsilon_c) = \frac{U \tilde{\eta}}{\Delta E_{\kappa'_2 \kappa_2 \kappa'_1 \kappa_1} - \epsilon_c} . \quad (9)$$

Here  $\tilde{\eta} = [1 - \eta(1 - 2\langle n_{i\uparrow} \rangle_0)(1 - 2\langle n_{i\downarrow} \rangle_0)]$ . The best values of  $\tilde{\eta}$  and  $\epsilon_c$  are determined again variationally.

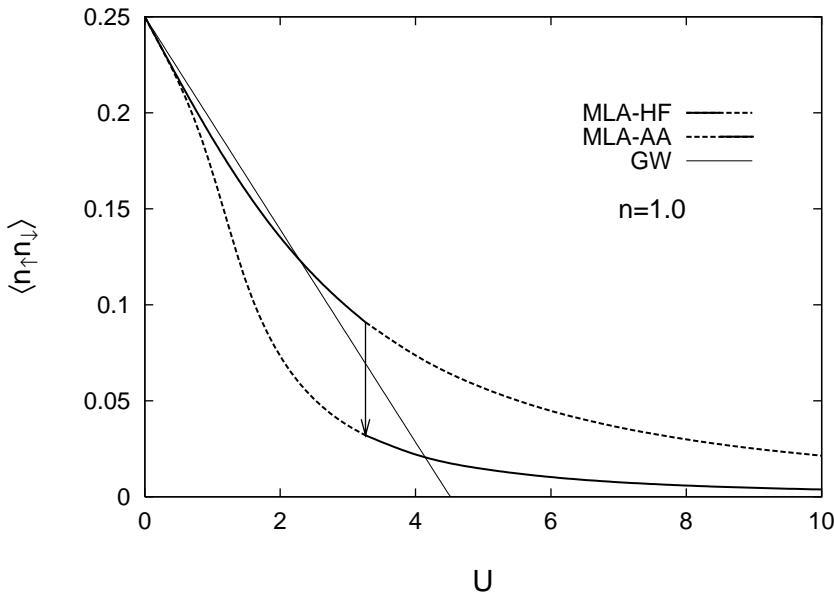
In the SSA, the correlation energy  $\epsilon_c$  can be expressed by the local density of states  $\rho_{i\sigma}(\epsilon)$  for the AA Hamiltonian (4). Because there is no translational symmetry due to random potential, we calculated  $\rho_{i\sigma}(\epsilon)$  by means of the Coherent Potential Approximation (CPA).<sup>23, 24)</sup>

To examine the validity of the MLA-AA as well as MLA-HF, we have performed the numerical calculations for the half-filled band Hubbard model with nearest neighbour transfer integral on the hypercubic lattice in infinite dimensions, where the SSA works best.<sup>25, 26)</sup> We assumed here the non-magnetic case. In this case, the density of states for non-interacting system is given by  $\rho(\epsilon) = (1/\sqrt{\pi}) \exp(-\epsilon^2)$ .<sup>25)</sup> The energy unit is chosen to be  $\int d\epsilon \rho(\epsilon) \epsilon^2 = 1/2$ . The characteristic band width  $W$  is given by  $W = 2$  in this unit.

Figure 1 shows the results of the ground-state energy vs Coulomb interaction energy curves. In the weak Coulomb interaction regime ( $U/W \lesssim 1$ ), the total energy of the MLA-HF is lower than the GW. On the other hand, we observe that the MLA-AA gives lower energy in comparison with the GW in the strong Coulomb interaction regime ( $U/W > 1$ ). We obtain the critical Coulomb interaction  $U_{c2} = 3.40$  at which the effective mass diverges. But before  $U$  approaches  $U_{c2}$  we find that the AA state showing the insulating state is stabilized, and the metal-insulator transition occurs at the critical Coulomb interaction  $U_c = 3.26$ . The transition is the first order in the present approach, and is consistent with the result of numerical renormalization group method (NRG), although the calculated  $U_{c2}$  is somewhat smaller than obtained by NRG (*i.e.*,  $U_{c2} = 4.1$

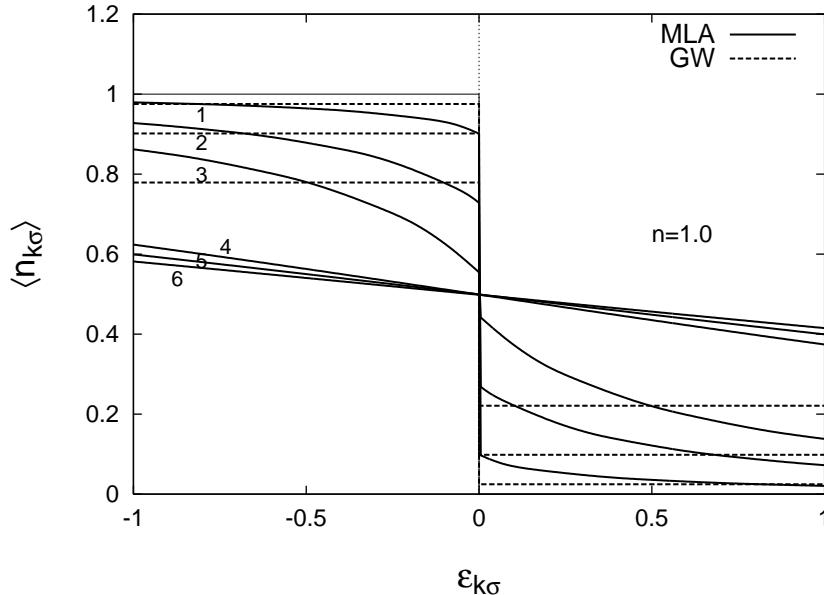


**Fig. 1.** The energy vs Coulomb interaction energy  $U$  curves in the MLA-AA (solid curve), MLA-HF (dashed curve), and GW (thin solid curve) for the electron number  $n = 1.0$ .



**Fig. 2.** The double occupation number  $\langle n_{\uparrow}n_{\downarrow} \rangle$  vs Coulomb interaction energy  $U$  curve for the electron number  $n = 1.0$  in the MLA-HF (solid-dashed curve), MLA-AA (dashed-solid curve), and GW (thin solid curve). The arrow shows a jump from the metallic state to the insulator at  $U_c = 3.26$ .

).<sup>27)</sup> The MLA-HF leads to the total energy lower than that of the GW up to the critical Coulomb interaction  $U_c$  and the MLA-AA gives the same behavior in the range  $U > U_c$ . More important is that the MLA scheme gives lower energy for overall Coulomb interaction regime and therefore can overcomes the limitation of the GW.



**Fig. 3.** The momentum distribution as a function of energy  $\epsilon_{k\sigma}$  for various Coulomb interaction energy parameters  $U = 1.0, 2.0, 3.0, 4.0, 5.0, 6.0$  at half-filling. The MLA: solid curve, the GW: dashed curve, and the HF: thin solid curve.

We present in Fig. 2 the double occupation number  $\langle n_\uparrow n_\downarrow \rangle$  as a function of Coulomb interaction energy  $U$  at half-filling. It decreases from  $1/4$  with increasing Coulomb interaction, so as to reduce the loss of Coulomb energy  $U$ . The MLA-HF state reduces more the double occupancy as compared with that of the GW in the weakly correlated region, and jumps to the MLA-AA state at  $U_c$ . In the strongly correlated regime, the MLA-AA gives finite value of double occupancy, while the GW gives the Brinkman-Rice atom. This verifies the improvement of the Brinkman-Rice atom. The double occupancy for the MLA scheme at  $U_c$  is 0.032, and is consistent with the result of the Quantum Monte Carlo ( $\approx 0.024$ ),<sup>28)</sup> though the latter uses the semi-elliptical density of states.

The momentum distribution for the MLA shows a clear momentum-dependence as a function of the HF one electron energy  $\epsilon_{k\sigma}$  as shown in Fig. 3. It decreases monotonically with increasing  $\epsilon_{k\sigma}$  and shows a jump at the Fermi energy. On the other hand, the distribution for the GW is constant below and above the Fermi level.<sup>1-3)</sup> The jump decreases with increasing  $U$ , and disappears beyond  $U_c$ , indicating the insulating state. The curve becomes flatter with further increase of  $U$ .

In summary, we have proposed a new momentum-dependent local ansatz wavefunction (MLA) which allows us to describe electron correlations starting from both the Hartree-Fock (HF) and the alloy-analogy (AA) limits. The former (*i.e.*, MLA-HF) de-

scribes the Fermi-liquid state, while the latter (*i.e.*, MLA-AA) describes the insulator state. We have performed the numerical calculations for the half-filled band Hubbard model on the hypercubic lattice in infinite dimensions, and demonstrated that the ground state energy for the MLA is lower than the GW in the whole range of Coulomb interaction. The MLA yields the metal-insulator transition at  $U_c = 3.26$ . The double occupation number is suppressed in the weak and intermediate Coulomb interaction regimes as compared with the GW, jumps at  $U_c$ , and remains finite in the strongly correlated regime as it should be. Finally, we found the momentum distribution functions showing a distinct momentum dependence in both the metallic and insulator regimes. These results indicate that the MLA approach can overcome the limitations of the original MLA, and goes beyond the GW in both the weak and strong  $U$  regimes.

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